

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
 Data File : BF127207.D
 Acq On : 04 Mar 2022 18:14
 Operator : CG\JU
 Sample : N1793-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-7

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.099	475	478	484	rVB	61118	64798	1.87%	0.330%
2	5.504	543	547	556	rBV	1146964	1128866	32.55%	5.746%
3	6.504	713	717	732	rVB	575896	685265	19.76%	3.488%
4	6.875	776	780	784	rBV	724520	575308	16.59%	2.928%
5	7.022	801	805	814	rBV	443442	390543	11.26%	1.988%
6	7.440	871	876	879	rBV	1863069	1948181	56.18%	9.916%
7	7.610	900	905	908	rVB	37533	37330	1.08%	0.190%
8	8.063	978	982	991	rBV	25947	61438	1.77%	0.313%
9	8.157	994	998	1002	rVV	867117	772803	22.29%	3.933%
10	9.234	1176	1181	1185	rBV	3334447	3467748	100.00%	17.650%
11	9.916	1288	1297	1301	rBV2	981082	998843	28.80%	5.084%
12	10.316	1360	1365	1367	rBV	36972	38326	1.11%	0.195%
13	10.716	1425	1433	1436	rBV	2298904	2311147	66.65%	11.763%
14	11.351	1538	1541	1544	rBV	51967	45699	1.32%	0.233%
15	11.410	1547	1551	1554	rBV	1105444	897982	25.90%	4.571%
16	11.569	1573	1578	1583	rBV3	24502	37303	1.08%	0.190%
17	11.792	1612	1616	1619	rBV	784562	622209	17.94%	3.167%
18	11.822	1619	1621	1624	rVB	50692	41629	1.20%	0.212%
19	12.998	1817	1821	1824	rBV	3415410	3297021	95.08%	16.781%
20	13.922	1974	1978	1981	rVB	53009	53079	1.53%	0.270%
21	13.992	1982	1990	1992	rBV4	57276	139275	4.02%	0.709%
22	14.057	1997	2001	2005	rVB	821061	707422	20.40%	3.601%
23	14.151	2011	2017	2023	rBV	360023	384978	11.10%	1.959%
24	14.822	2126	2131	2135	rBV2	69597	86706	2.50%	0.441%
25	15.163	2185	2189	2193	rVB2	52012	62754	1.81%	0.319%
26	15.545	2249	2254	2262	rBV	512880	624569	18.01%	3.179%
27	15.992	2326	2330	2337	rVB	45349	74115	2.14%	0.377%
28	16.510	2414	2418	2424	rBV2	31149	51916	1.50%	0.264%
29	17.121	2518	2522	2529	rVB6	21114	39927	1.15%	0.203%

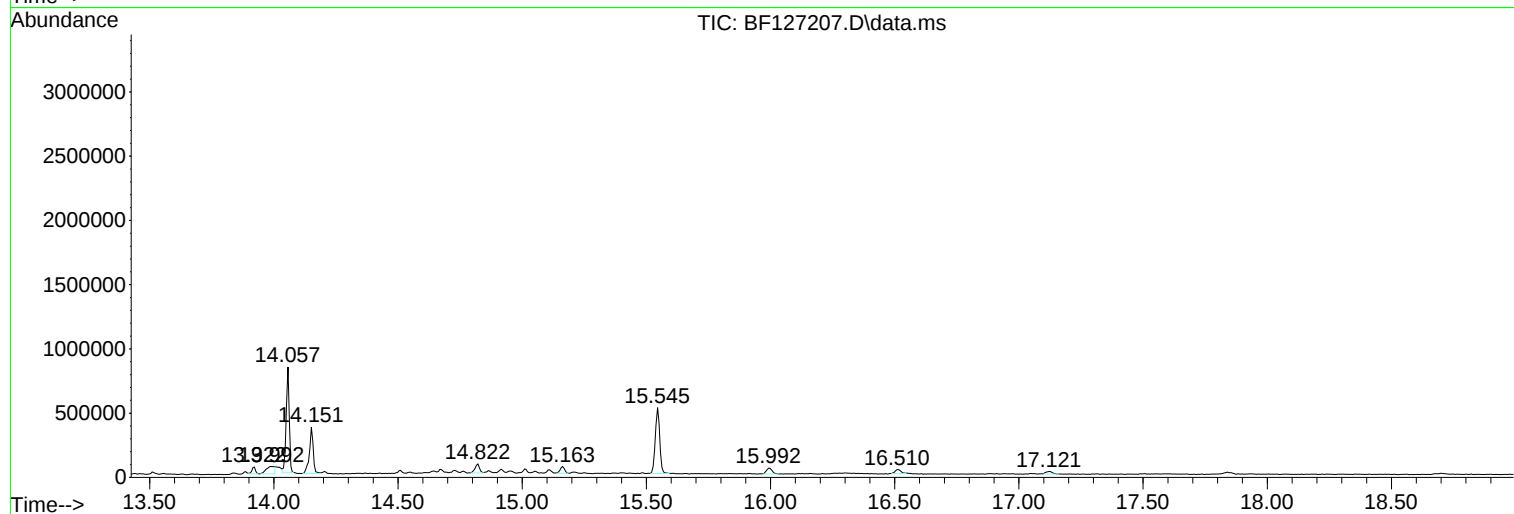
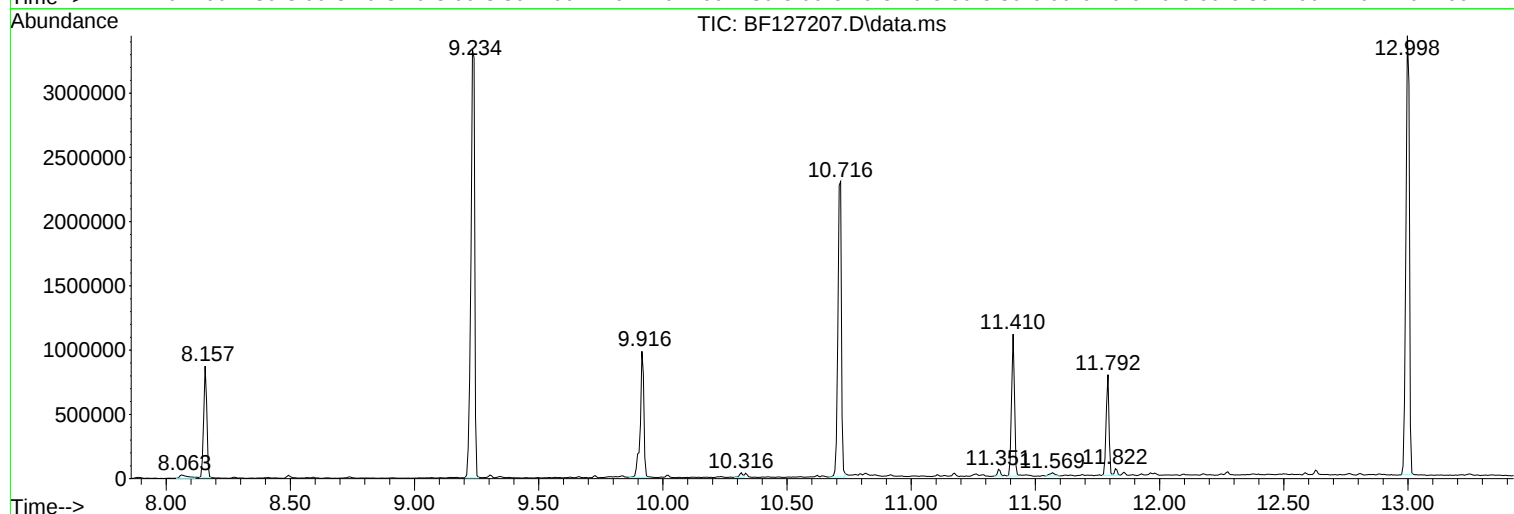
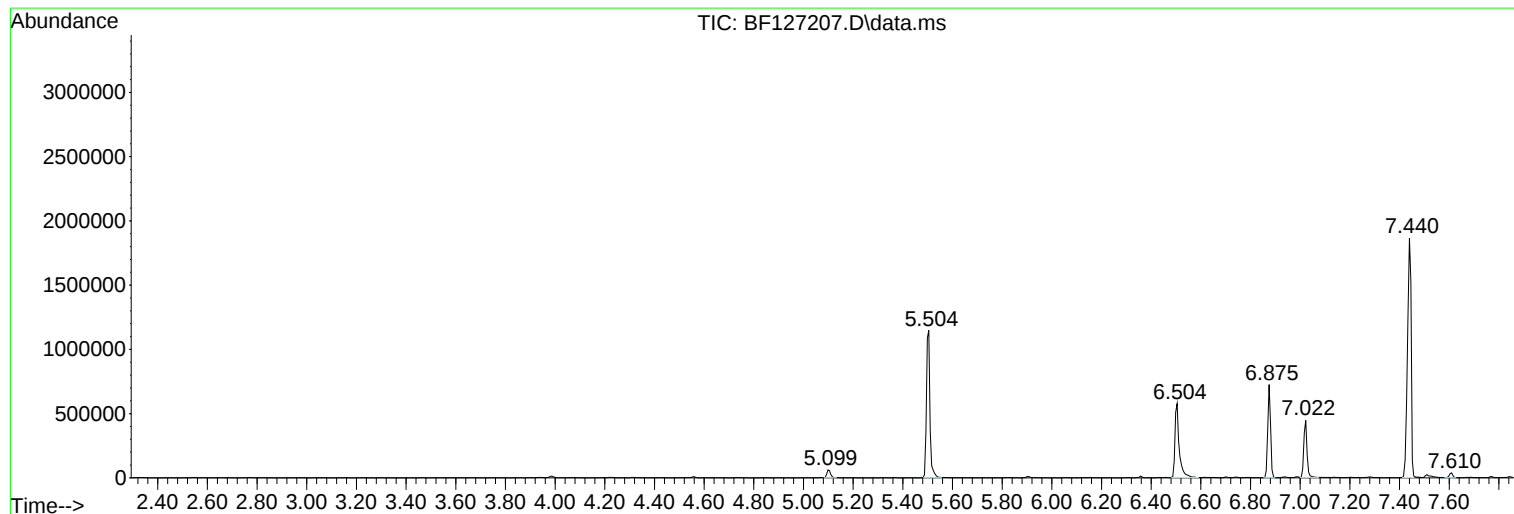
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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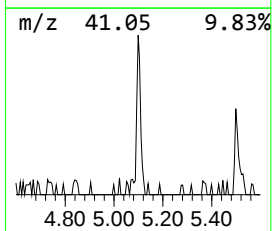
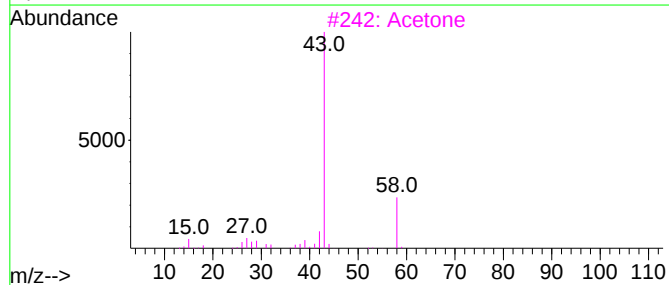
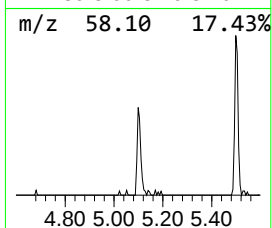
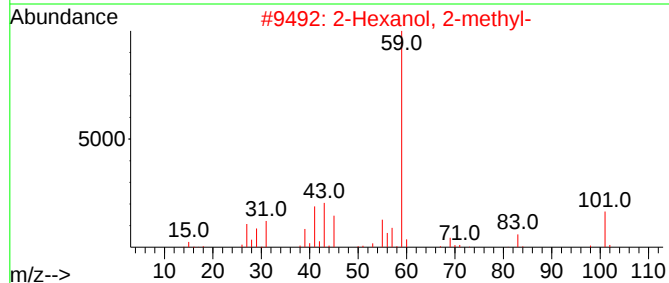
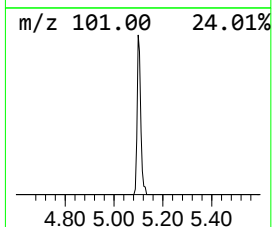
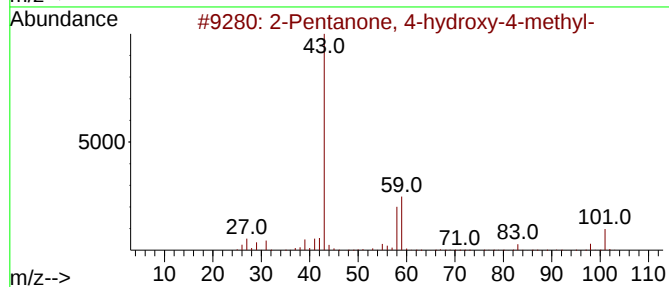
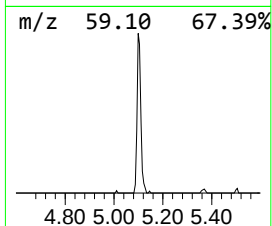
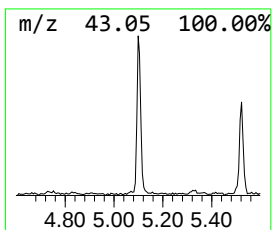
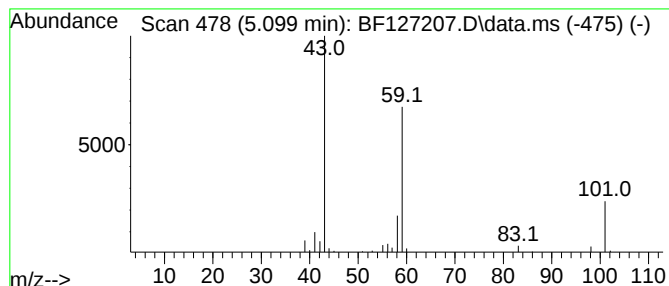
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	2.25 ng	64798	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3		Acetone	58	C3H6O	000067-64-1	9
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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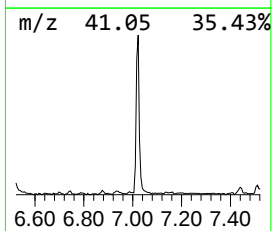
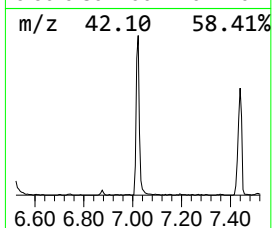
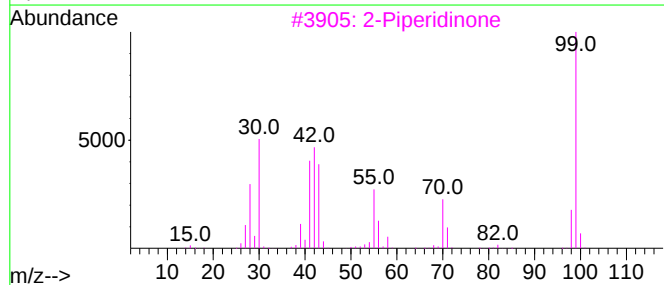
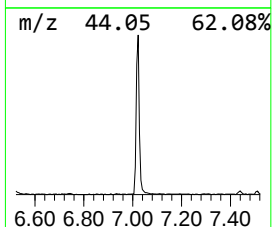
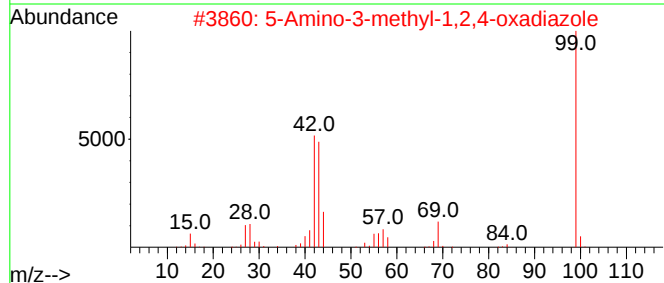
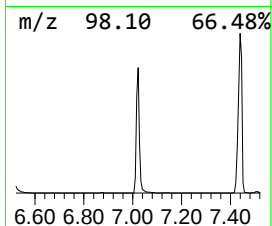
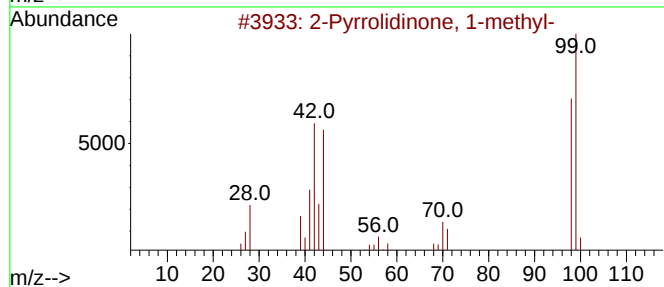
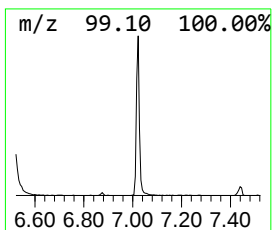
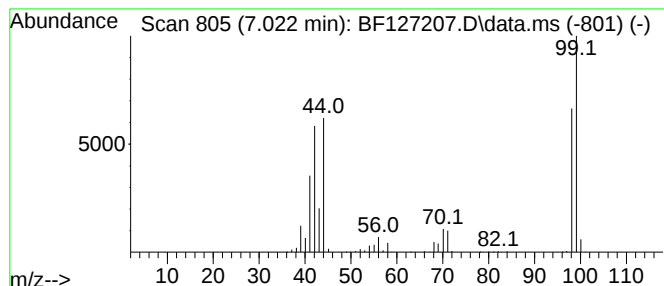
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.022	13.58 ng	390543	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	95
2			5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	43
3			2-Piperidinone	99	C5H9NO	000675-20-7	37
4			5-Aminopentanamide	116	C5H12N2O	013023-70-6	33
5			Allyl Isothiocyanate	99	C4H5NS	000057-06-7	32



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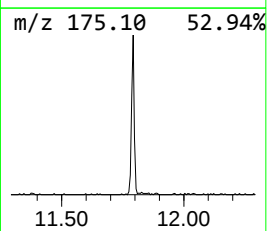
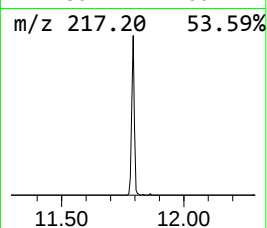
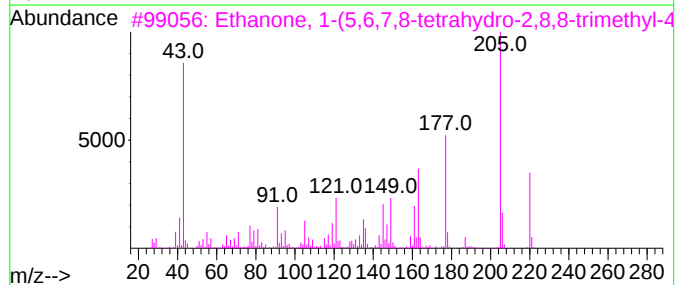
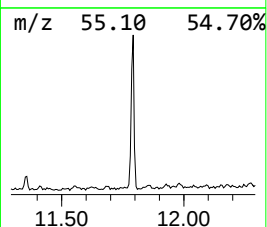
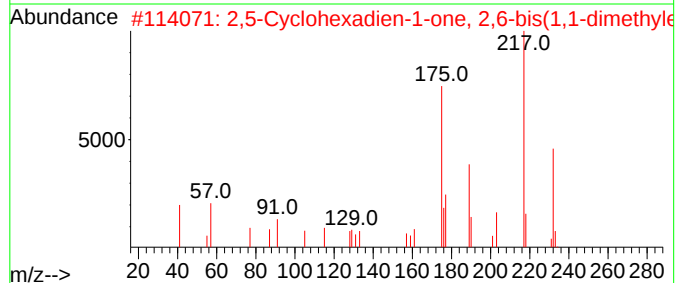
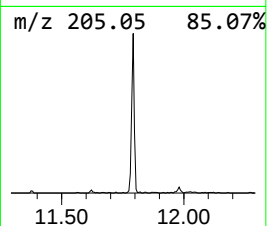
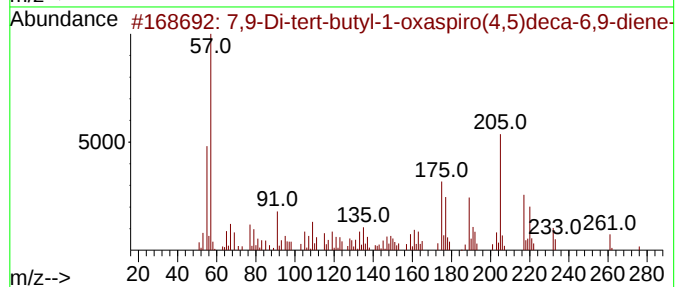
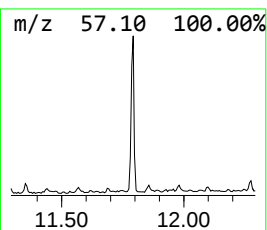
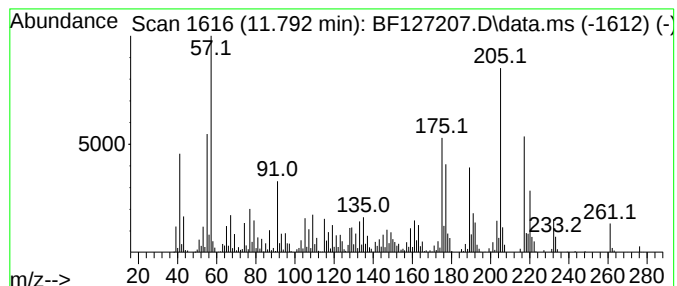
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.792	13.86 ng	622209	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	99
2	2,5-Cyclohexadien-1-one, 2,6-bis...		232	C16H24O	006738-27-8	83
3	Ethanone, 1-(5,6,7,8-tetrahydro-...		220	C14H20O2	071596-88-8	50
4	1-(3-Amino-4,6-dimethylthieno[2,...		220	C11H12N2OS	052505-42-7	50
5	(Z)-((2-Benzylideneheptyl)oxy)tr...		276	C17H28OSi	1000495-65-9	45



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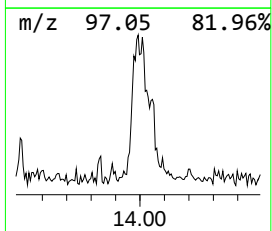
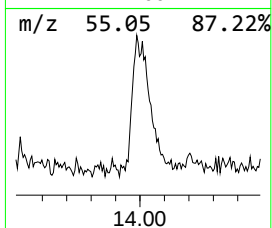
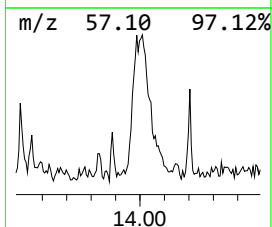
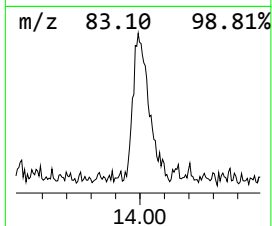
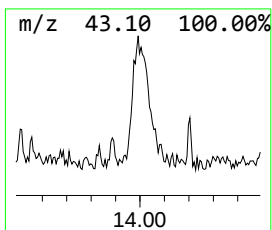
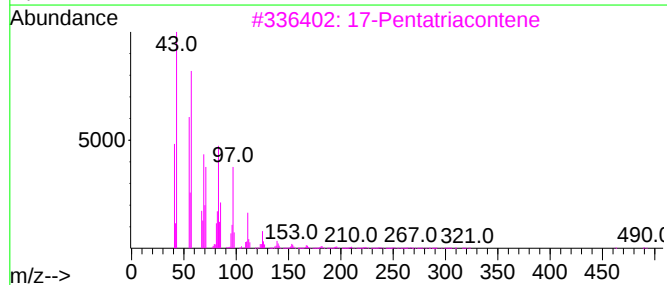
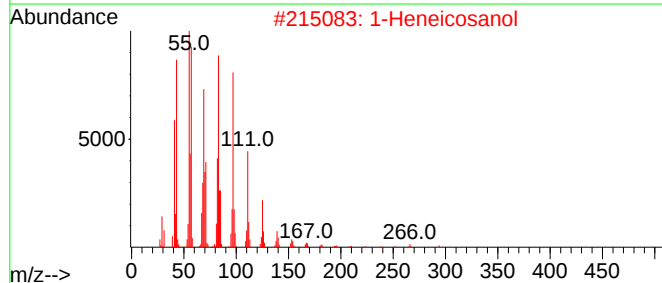
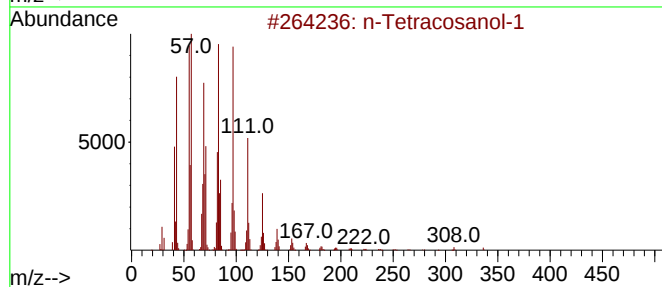
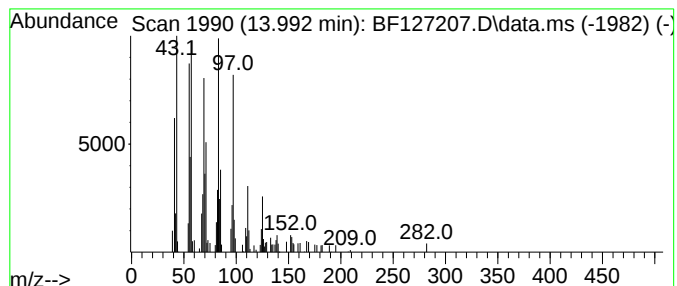
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	3.94 ng	139275	Chrysene-d12	14.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2		1-Heneicosanol	312	C21H44O	015594-90-8	83
3		17-Pentatriacontene	491	C35H70	006971-40-0	83
4		1-Tetracosene	336	C24H48	010192-32-2	83
5		1-Tricosene	322	C23H46	018835-32-0	76



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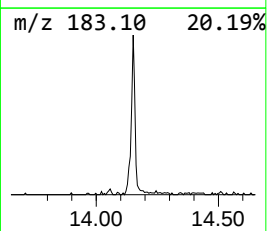
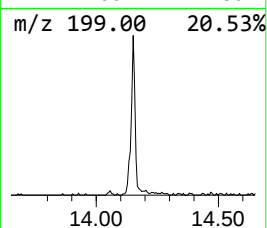
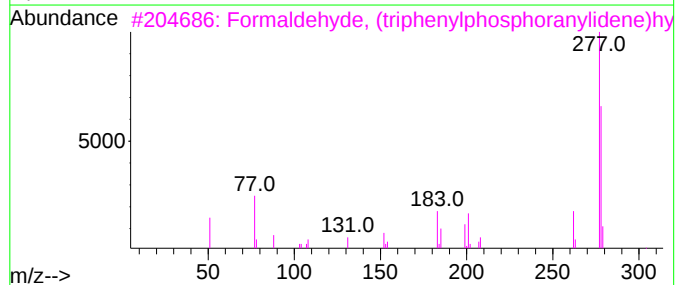
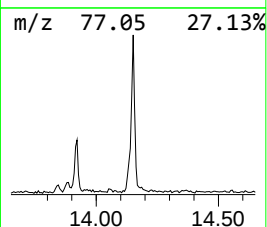
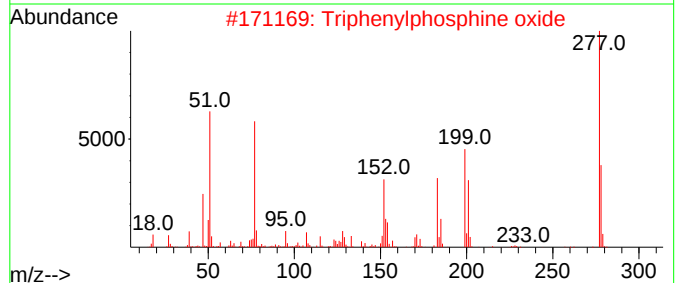
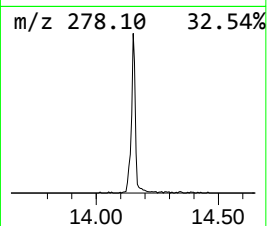
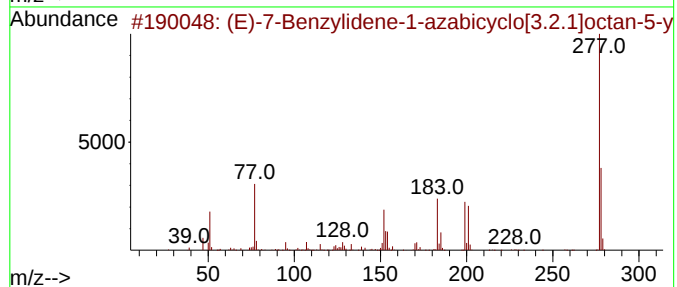
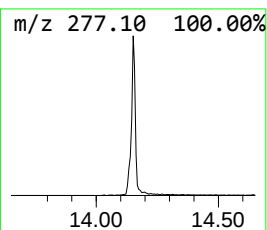
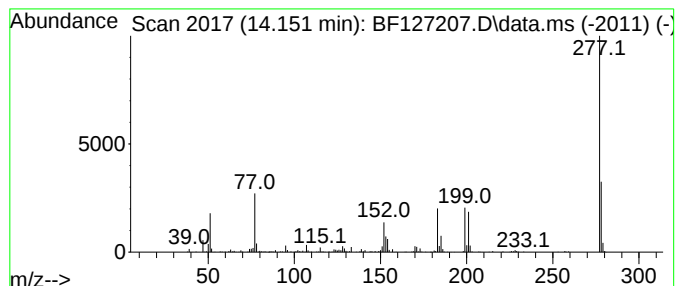
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Peak Number 5 (E)-7-Benzylidene-1-azabicy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	10.88 ng	384978	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64		
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38		
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25		



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SB-7

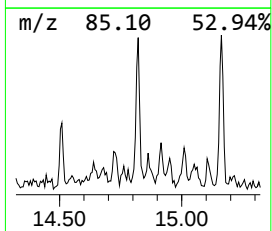
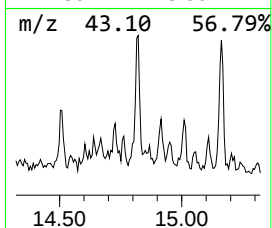
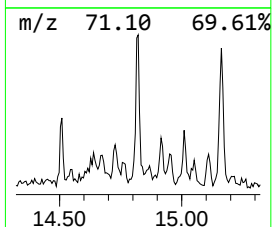
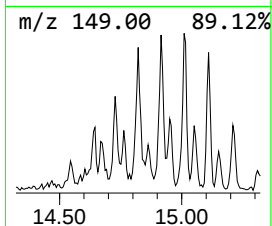
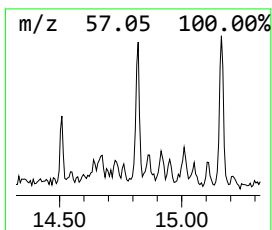
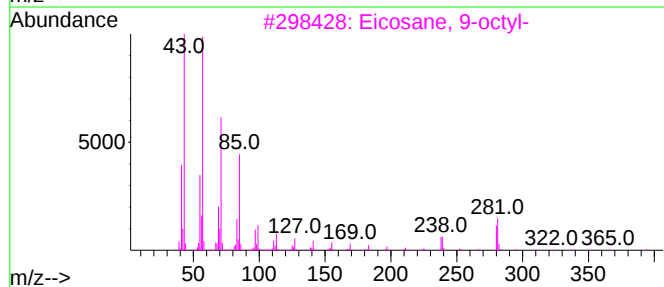
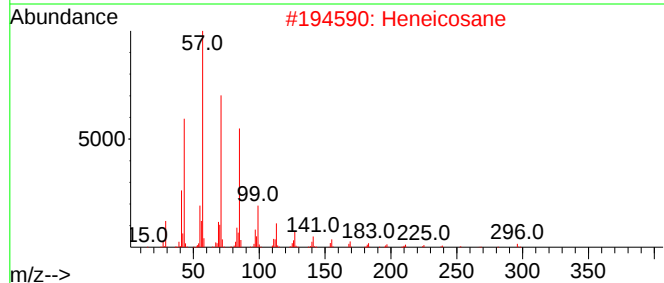
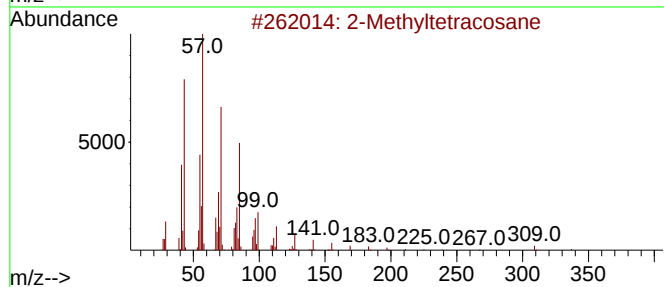
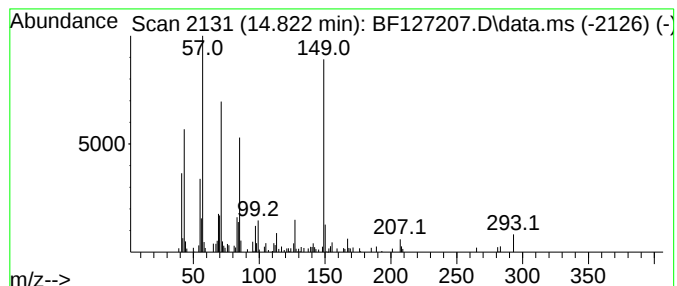
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.822 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.822	2.78 ng	86706	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methyltetracosane	352	C25H52	001560-78-7	49
2		Heneicosane	296	C21H44	000629-94-7	49
3		Eicosane, 9-octyl-	394	C28H58	013475-77-9	46
4		Hexacosane	366	C26H54	000630-01-3	46
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127207.D
Acq On : 04 Mar 2022 18:14
Operator : CG\JU
Sample : N1793-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7

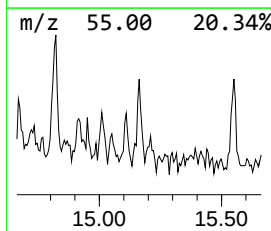
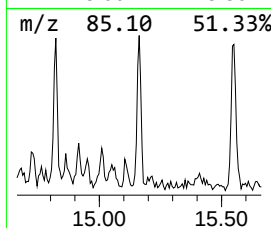
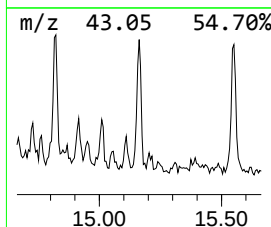
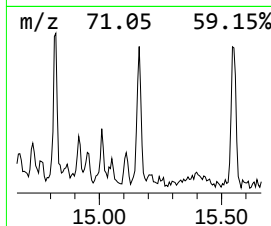
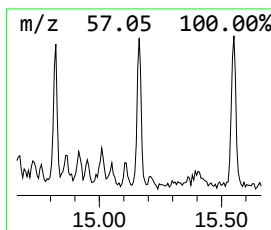
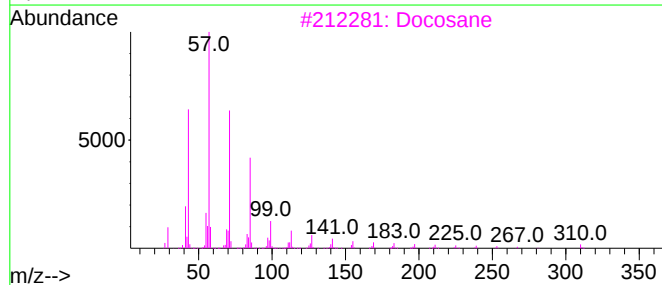
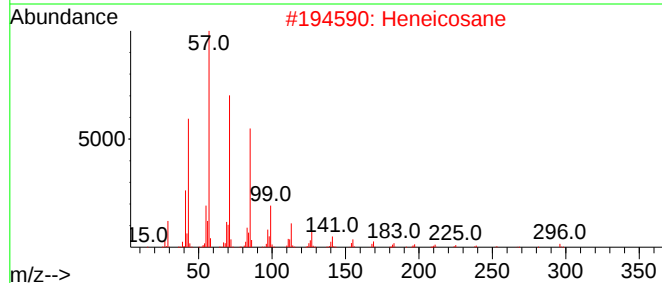
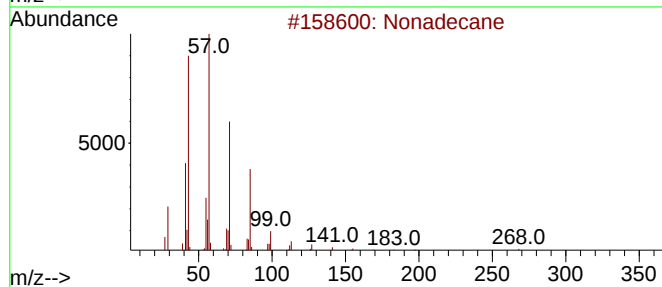
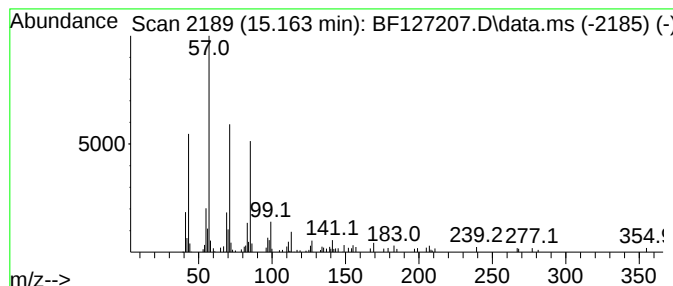
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.01 ng	62754	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Docosane	310	C22H46	000629-97-0	87
4			Heptadecane	240	C17H36	000629-78-7	87
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127207.D
Acq On : 04 Mar 2022 18:14
Operator : CG\JU
Sample : N1793-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7

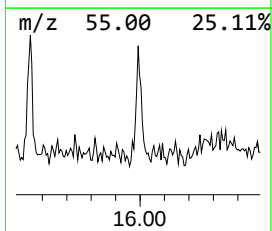
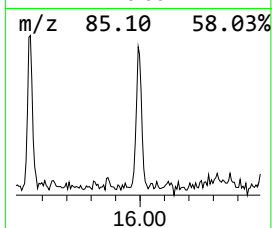
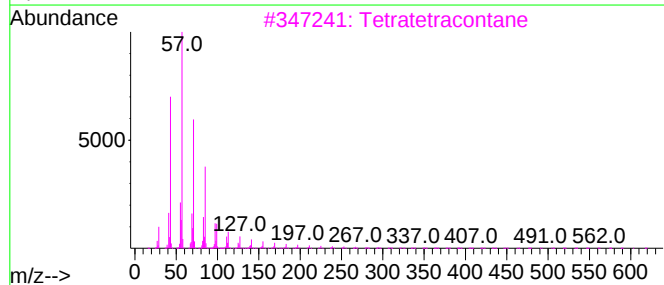
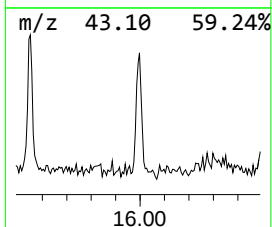
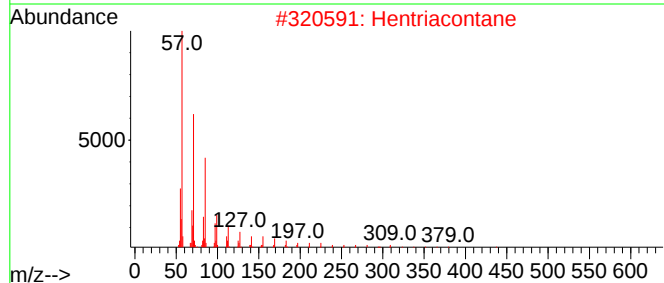
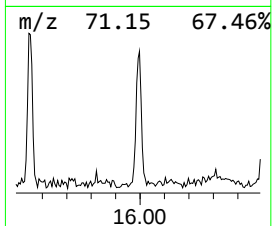
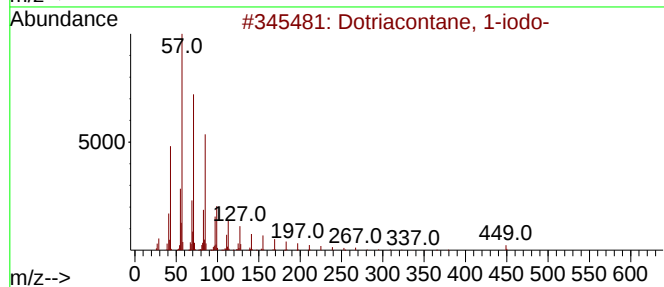
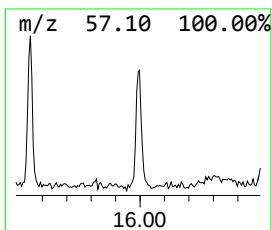
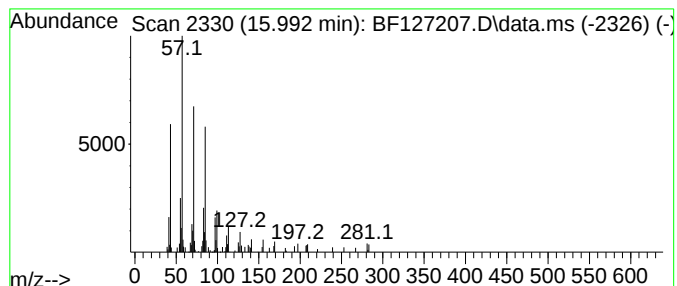
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dotriacontane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	2.37 ng	74115	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127207.D
Acq On : 04 Mar 2022 18:14
Operator : CG\JU
Sample : N1793-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.099	2.3	ng	64798	1	6.875	575308	20.0
2-Pyrrolidinone...	7.022	13.6	ng	390543	1	6.875	575308	20.0
7,9-Di-tert-but...	11.792	13.9	ng	622209	4	11.410	897982	20.0
n-Tetracosanol-1	13.992	3.9	ng	139275	5	14.057	707422	20.0
(E)-7-Benzylide...	14.151	10.9	ng	384978	5	14.057	707422	20.0
unknown14.822	14.822	2.8	ng	86706	6	15.545	624569	20.0
Nonadecane	15.163	2.0	ng	62754	6	15.545	624569	20.0
Dotriacontane, ...	15.992	2.4	ng	74115	6	15.545	624569	20.0